2-BROMOBENZYL BROMIDE

Other names:	o-Bromobenzyl bromide
	2-Bromobenzyl bromide
	«alpha»-2-dibromotoluene
Inchi:	InChI=1S/C7H6Br2/c8-5-6-3-1-2-4-7(6)9/h1-4H,5H2
InchiKey:	LZSYGJNFCREHMD-UHFFFAOYSA-N
Formula:	C7H6Br2
SMILES:	BrCc1ccccc1Br
Mol. weight [g/mol]:	249.93

Physical Properties

Property code	Value	Unit	Source
hf	86.38	kJ/mol	Cheméo Relay (1.0)
hfus	18.11	kJ/mol	Joback Method
hvap	62.72	kJ/mol	Cheméo Relay (1.0)
ie	9.00	eV	Cheméo Relay (1.0)
log10ws	-3.66		Cheméo Relay (1.0)
logp	3.344		Crippen Method
mcvol	120.730	ml/mol	McGowan Method
tb	526.45	K	Cheméo Relay (1.0)
tf	304.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.04	J/mol×K	523.54	Joback Method
cpg	213.54	J/mol×K	565.41	Joback Method
cpg	222.25	J/mol×K	607.29	Joback Method
cpg	230.24	J/mol×K	649.16	Joback Method
cpg	237.56	J/mol×K	691.03	Joback Method
cpg	244.28	J/mol×K	732.90	Joback Method
cpg	250.46	J/mol×K	774.78	Joback Method
dvisc	0.0018542	Pa×s	327.19	Joback Method
dvisc	0.0012150	Pa×s	359.91	Joback Method
dvisc	0.0008542	Pa×s	392.64	Joback Method

dvisc	0.0006340	Pa×s	425.37	Joback Method
dvisc	0.0004911	Pa×s	458.09	Joback Method
dvisc	0.0003935	Pa×s	490.81	Joback Method
dvisc	0.0003242	Pa×s	523.54	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	402.20	K	2.50	NIST Webbook
tbrp	418.00 ± 2.00	K	3.30	NIST Webbook
tbrp	398.00 ± 5.00	K	1.70	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3433805&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure

tf: Normal melting (fusion) point